WHAT IS CLAIMED:

1. A method, comprising the steps of:

providing a first molecule;

decomposing the molecule into two or more molecular fragments; and

introducing one or more pairs of conjugated caps having a first cap member and a second cap member at one or more locations in the molecule to create a plurality of molecular portions, wherein each molecular portion comprises a fragment of the first molecule and at least one of the first and second cap members of at least one pair of conjugated caps.

2. The method as set forth in claim 1, wherein the providing step comprises electronically generating the first molecule.

3. The method as set forth in claim 2, wherein the decomposing step comprises electronically cutting the molecule.

4. The method as set forth in claim 3, wherein the introducing step comprises electronically introducing the one or more pairs of conjugated caps into the electronically generated first molecule.

5. The method as set forth in claim 1, further comprising the step of

calculating an intermolecular interaction energy between the first molecule and a second molecule based on the plurality of molecular portions.

6. The method as set forth in claim 5, wherein the calculating step comprises determining an interaction energy between each of the molecular portions and the second molecule.

7. The method as set forth in claim 6, wherein the calculating step comprises at least one first computing system calculating an interaction energy between a first molecular portion and the second molecule, and a second computing system

calculating the interaction energy between a second molecular portion and the second molecule.

8. The method as set forth in claim 6, further comprising the step of

summing together the interaction energies determined for each of the molecular portions and the second molecule to provide a total interaction energy of the molecular portions.

9. The method as set forth in claim 8, further comprising the step of

summing together one or more conjugated cap interaction energies obtained from each of the one or more pairs of conjugated caps and the second molecule to provide a total conjugated cap interaction energy; and

subtracting the total conjugated cap interaction energy from the total interaction energy of the molecular portions to provide an intermolecular interaction energy between the first molecule and the second molecule.

10. The method as set forth in claim 9, wherein the intermolecular interaction energy is a quantum mechanical intermolecular interaction energy.

11. The method as set forth in claim 1, wherein the first molecule is a polyatomic species.

12. The method as set forth in claim 11, wherein the polyatomic species is selected from the group consisting of a material, a protein, a peptide, a polymer, DNA, and RNA.

13. The method as set forth in claim 1, wherein the second molecule is selected from the group consisting of an ion, a water molecule, an inorganic molecule, an organic molecule, a drug molecule, and a biological molecule.

14. The method as set forth in claim 1, wherein the first molecule is a protein or a peptide and the second molecule is a drug molecule.

15. The method as set forth in claim 1, wherein the first and second cap members are independently selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

16. A computer-readable medium having stored thereon instructions for calculating an intermolecular interaction energy, said instructions comprising:

instructions for providing a first molecule;

instructions for decomposing the first molecule into two or more molecular fragments; and

instructions for introducing one or more pairs of conjugated caps having a first cap member and a second cap member at one or more locations in the first molecule to create a plurality of molecular portions, wherein each molecular portion comprises a fragment of the first molecule and at least one of the first and second cap members of at least one pair of conjugated caps.

17. The medium as set forth in claim 16, further comprising

instructions for calculating an intermolecular interaction energy between the first molecule and a second molecule based on the plurality of molecular portions.

18. The medium as set forth in claim 17, wherein said instructions for calculating comprise instructions for determining an interaction energy between each of the molecular portions and the second molecule.

19. The medium as set forth in claim 18, wherein said instructions for determining an interaction energy include instructions for calculating an interaction energy between a first molecular portion and the second molecule, and instructions for calculating an interaction energy between a second molecular portion and the second molecule.

20. The medium as set forth in claim 18, further comprising

instructions for summing together the interaction energies determined for each of the molecular portions and the second molecule to provide a total interaction energy of the molecular portions.

21. The medium as set forth in claim 20, further comprising

instructions for summing together one or more conjugated cap interaction energies obtained from each of the one or more pairs of conjugated caps and the second molecule to calculate a total conjugated cap interaction energy; and

instructions for subtracting the total conjugated cap interaction energy from the total interaction energy of the molecular portions to provide an intermolecular interaction energy between the first molecule and the second molecule.

22. The medium as set forth in claim 21, wherein the intermolecular interaction energy is a quantum mechanical intermolecular interaction energy.

23. The medium as set forth in claim 16, wherein the first molecule is a polyatomic species.

24. The medium as set forth in claim 19, wherein the polyatomic species is selected from the group consisting of a material, a protein, a peptide, a polymer, DNA, and RNA.

25. The medium as set forth in claim 17, wherein the second molecule is selected from the group consisting of an ion, a water molecule, an inorganic molecule, an organic molecule, a drug molecule, and a biological molecule.

26. The medium as set forth in claim 16, wherein the first and second cap members are selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

27. A system for calculating an intermolecular interaction energy, the system comprising:

a molecular generation module that provides a first molecule;

a molecular decomposition module that decomposes the molecule into two or more molecular fragments; and

a molecular cap introduction module that introduces one or more pairs of conjugated caps having a first cap member and a second cap member at one or more locations in the first molecule to create a plurality of molecular portions, wherein each molecular portion comprises a fragment of the first molecule and one of the first and second cap members of at least one pair of conjugated caps.

28. The system as set forth in claim 27, further comprising

an energy calculation module that calculates the molecular interaction energy between the first molecule and a second molecule based on the plurality of molecular portions.

29. The system as set forth in claim 28, wherein the energy calculation module determines the interaction energy between each of the molecular portions and the second molecule.

30. The system as set forth in claim 29, wherein the energy calculation module comprises at least one first computing system that calculates an interaction energy between a first molecular portion and the second molecule, and at least one second computing system that calculates an interaction energy between a second molecular portion and the second molecule.

31. The system as set forth in claim 29, wherein the energy calculation module sums together the interaction energies determined for each of the molecular portions and the second molecule to provide a total interaction energy of the molecular portions.

32. The system as set forth in claim 31, wherein the molecular interaction energy module

sums together one or more conjugated cap interaction energies obtained from each of the one or more pairs of conjugated caps and the second molecule to provide a total conjugated cap interaction energy; and

subtracts the total conjugated cap interaction energy from the total interaction energy of the molecular portions to provide an intermolecular interaction energy between the first molecule and the second molecule.

33. The system as set forth in claim 32, wherein the intermolecular interaction energy is a quantum mechanical intermolecular interaction energy.

34. The system as set forth in claim 27, wherein the first molecule is a polyatomic species.

35. The system as set forth in claim 34, wherein the polyatomic species is selected from the group consisting of a material, a protein, a peptide, a polymer, DNA, and RNA.

36. The system as set forth in claim 27, wherein the second molecule is selected from the group consisting of an ion, a water molecule, an inorganic molecule, an organic molecule, a drug molecule, and a biological molecule.

37. The system as set forth in claim 27, wherein the first molecule is a protein or a peptide and the second molecule is water.

38. The system as set forth in claim 27, wherein the first and second cap members are selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

39. A composition comprising:

a molecule comprising a plurality of units, and

a plurality of pairs of conjugated caps having a first cap member and a second cap member, wherein each of the plurality of pairs of conjugated caps is inserted between two of the plurality of units under conditions effective to substantially preserve the properties of a chemical bond being cut to insert the pair of conjugated caps and wherein the first cap member substantially mimics the electronic effect of the units of the molecule on a first side of the pair of conjugated caps and the second cap member substantially mimics the electronic effect of the units of the molecule on a second side of the pair of conjugated caps.

40. The composition as set forth in claim 39, wherein the pairs of conjugated caps form molecular species.

41. The composition as set forth in claim 39, where the molecule comprises two or more units.

42. The composition as set forth in claim 39, wherein the molecule is selected from the group consisting of a protein, a peptide, a polymer, DNA, and RNA.

43. The composition as set forth in claim 39, wherein the first and second cap members are selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

44. The composition as set forth in claim 39, wherein at least two of the molecular fragments in the molecule are fused together through the molecular caps.